Using Higher-Order Derivatives to Estimate Damped Linear Oscillator

Models with an Over-Arching Temporal Trend

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Abstract

Studies that look to examine intra-individual data have become more popular in the social sciences in recent years, and thusly methods that accurately model this type of data are needed. One particular differential equation model that has been used to fit this type of data is the damped linear oscillator (DLO), which models constructs that vary about some equilibrium value over time. Currently, methods for fitting the DLO model require that no over-arching, temporal trend be present in the data, or that this trend be removed prior to fitting the model in some two-step procedure. One such two-step approach that has been used in psychology is the method of Latent Differential Equations (LDE). Using two-step procedures can cause standard errors of parameter estimates to be inflated, which makes single-step methods with simultaneous estimation of all parameters preferred. This study proposes a method using higher-order derivatives and structural equation modeling (SEM) to estimate the DLO model and trend simultaneously. A simulation was conducted to examine (a) the bias of estimates obtained using the proposed method and (b) whether the proposed method provides any improvement over the existing, two-step LDE approach. The results suggest that the proposed method does provide accurate estimates, but for a much smaller range of conditions than the LDE approach. The simultaneous estimation of the higher-order derivative method did provide more precise parameter estimates compared to the two-step approach for the range of conditions that it was found to be accurate.

Keywords: damped linear oscillator, derivative, dynamical systems

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Table of Contents

List of Tables & Figures

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Background and Theory

Over the last couple of decades, a shift has been occurring in the social sciences towards trying to design studies that more closely parallel real world phenomena. A specific result of this ideological change is that many researchers now look at their area of interest as an ever-changing series of interacting factors. While some traditional methods, such as growth curve modeling, can be applied in some of these settings, in an attempt to keep-up with these advances in experimental design, various methods have been designed to better analyze the kind of data that comes from these types of studies. One of the more recent additions to this arsenal of methodologies is the area of dynamical systems.

Growth curve modeling utilizes the flexible framework of structural equation modeling (SEM) to analyze longitudinal data (Kline, 2010). These models allow for linear, quadratic, and theoretically even higher-order trends to be fit to data to examine how a variable changes over time. Once a temporal trend has been fit to the data, it can then be used to make inferences about the group of participants as a whole. These models are very useful in many studies, but they do have some drawbacks that limit their applicability in some situations. One major limitation is that only low-order, polynomial trends can typically be fit, and although more complex trends could be fit theoretically, doing so in an interpretable manner is often very difficult in practice. A second major limitation is that inferences are made at the group level and, even though individual differences can be estimated, very little information can be gleaned about a particular individual. Multilevel modeling can be applied to growth curves to try to get individual-level data, but even though this method may be able to provide each individual's resultant curve, it does little in explaining what is actually happening among the variables within the system. For example, these models do not differentiate between whether an effect of a variable on an individual's curve is due to the exogenous event itself or the variable's interaction with the self-regulating dynamics of the individual (Curran, Stice, & Chassin, 1997). This can be an important distinction because people are, by nature, constantly regulating themselves.

Given these limitations of growth curve modeling, there are many experimental designs that would not be able to be analyzed using this method. One set of studies that require different approaches are those that are designed to look at rapidly changing, intra-individual data. *Intra-individual data* is data that looks at individuals as forever changing sets of traits that form an always evolving set of dynamic systems. Put simply, people are constantly changing (Baltes, Reese, & Nesselroade, 1977). Many studies are designed to look at how a given individual changes over time, and obviously not everyone matches the group average found in most traditional analysis methods. Additionally, intra-individual changes will not only impact that individual, but they can also indirect affect differences between-subjects (Boker, Leibenluft, Deboeck, Virk, & Postolache, 2008). For example, if a tragedy occurs and a person's mood is different from their "typical, baseline mood" at a given time, then this will also influence how this person compares to other individuals in the study at that point in time. So, although this individual may "typically" be close to the other subjects' moods, at this point in time they may be an extreme value that significantly impacts between-subject's estimates. A method that can capture these intra-individual changes, as well as overall trends, is necessary to get a more realistic depiction of what is happening in these data sets, and thus the real world. Dynamical systems models have been found to be very effective in analyzing data in these types of longitudinal studies (Boker et al., 2008; Boker & Graham, 1998; Bisconti, Bergeman, & Boker, 2006). These models have been found to be especially useful because they allow for a variable to evolve with respect to information from earlier points in time, while also accounting for the impact of factors that occur outside of the individual.

Before delving into the particular intricacies of dynamical systems models, it is important to define and discuss some terms and concepts that are common to the area of dynamical systems. For the purposes of this discussion, a *system* will be defined as the set of variables that make-up a given latent construct, or set of constructs. The *state* of a system is simply the set of values of all of the variables in the system at a specific point in time, t. A *dynamical system* is a system in which the state of the system at time, t, is to some degree dependent on the state of that system at time, $t-\tau$, for some length of time, τ. Given these definitions, many systems that are studied longitudinally are indeed dynamical systems (Boker & Nesselroade, 2002). In fact, it may even be difficult to find a system in which variables at a given point in time do not at all influence variables at subsequent time points. The widespread applicability of dynamical systems models is readily apparent given the diverse areas of the social sciences that have employed them (Boker et al., 2008; Boker & Graham, 1998; Bisconti et al., 2006).

The following sections will provide an overview of the evolution of one methodology for analyzing intra-individual variability. First, a brief discussion of growth curve modeling is given as it applies to dynamical systems methods. Following that, an introduction to dynamical systems models is provided, and finally the purpose of and need for the current study is described.

Growth Curve Models

Growth curve models are a very useful analysis method for studies that want to examine change over time that occurs slowly relative to the frequency that the data was collected. These models have been widely studied, and although a brief summary is given here, a more thorough discussion of their theory and application can be found elsewhere (Kline, 2010; Bollen & Bollen, 1989). This method serves as a suitable beginning for a discussion on dynamical systems for multiple reasons. Firstly, the need that dynamical systems models fill is easy to present/understand by framing it in terms of the more widely known concepts of growth curve modeling. Also, the ideas employed by some dynamical systems methods, including the method that is presented in this study, are quite similar to those found in growth curve modeling, so an understanding of one can aid in learning about the other.

Growth curve models are designed to look at an overall trend in variables over time. Although they are designed to look at between-subjects type change, they can be modified to allow for some within-subjects inferences to be made by applying multilevel modeling (Raudenbush & Bryk, 2001), which is necessary to be applicable to studies that look at intra-individual data. These multilevel models can be used to find the trend that each individual follows over the course of a study. Other than the geometrically simple, over-arching trend however, there is not much more that these models explain about how an individual's construct varies about the overall trend. Do they move about it quickly? Slowly? Evenly? In studies of intra-individual data, these are questions that may be of interest. There are two additional limitations to fitting models to intra-individual data using traditional methods that will be discussed in more detail, as they are more relevant to the area of dynamical systems. They are the "phase problem" and the "sampling interval problem" (Boker & Nesselroade, 2002).

The "phase problem" is most easily presented and understood through an example. Consider a study that is looking at individuals' moods at two time points, once as they first arrive for the study and the second after watching public television for one hour. If people are selected randomly, and assuming peoples' moods vary over time with some set of dynamics, the participants will have some random distributions of moods at the first time point (i.e., some may have encountered bad traffic; some may have found a twenty dollar bill on the sidewalk). Thusly, after the participants watch television for an hour, they have some probability to have their mood improve or decline. It is possible though, that this is not an effect of watching an hour of television, as much as it is an effect of people beginning at different moods. There would be no way for the analyst to parse out the effect of watching television from peoples' differing initial moods using traditional methods. It could be that every subject enjoyed watching television, but the effect was washed out by the effects of their initial differences (Boker & Nesselroade, 2002).

The above scenario is an example that indicates how problematic the "phase problem" can be for growth curve modeling and other traditional analysis methods. If subjects are at different levels of a variable at the beginning of a study, this variability in initial conditions can alter the results of the analyses and could thusly hurt the validity of the study. This is a major issue since it is often very difficult to determine a given individual's initial level on a given variable, and it would be even more difficult to collect data only on individuals with similar initial states. Dynamical systems models however, are not hindered by this problem. Dynamical systems models attempt to reconstruct the phase space of each individual, which is a way of accounting for differences in the starting points of various individuals' initial values, while still extracting the desired information regarding the intra-individual dynamics for each subject (Boker & Bisconti, 2006).

The second issue that merits further mentioning is not necessarily an issue of growth curves (although it could be), but it is an issue for modeling intra-individual dynamics. This issue is known as the “measurement interval problem”. This problem gets at the question of what the most appropriate sampling interval is for any given study. An interval that is too long risks “jumping over” information that is relevant to the study, while a sampling interval that is too short will be overly sensitive to random error, or noise, in the data. Although this is still an issue that must be examined when applying dynamical systems models, there are algorithms that allow for the calculation of the optimal sampling interval (Boker & Nesselroade, 2002).

Dynamical Systems Models

The definition of a dynamical system states that the values of a variable(s) at a given time point is at least partially informed by values at some previous time point(s). A set of systems that behave under this assumption are self-regulating systems. *Self-regulation* is a process by which the value and rate of change of a variable are used to inform future values of that variable (Carver & Scheier, 1998). The variable is self-regulating in that it uses its own values to propagate itself.

A simple example of a self-regulating system is a thermostat regulating the temperature of a room. For example, if the thermostat for a heater is set at seventy degrees, this makes it so the heater will begin running if the temperature in the room drops below seventy degrees. The heater will continue to run until the temperature in the room exceeds seventy degrees. Also, assume that the thermostat causes the heater to produce less heat the faster the temperature in the room is changing, so as to not heat the room well past seventy degrees. So, even though the thermostat is set at one specific value, the actual temperature of the room oscillates up and down around that value. The system is completely governed by the temperature and how fast the temperature is changing at any given time. This type of system has been applied in many areas of psychology including mood, depression, and substance abuse (Boker et al., 2008; Bisconti et al., 2004; Boker & Graham, 1998). Since self-regulating systems are a class of dynamical systems used frequently in the social sciences, they will be the focus of the remainder of this paper.

Within the social sciences the application of dynamical systems models has been limited to only a few models, and one of these models is the damped linear oscillator model (Hubbard & West, 1991). Due to its widespread use, this model will be used throughout the following discussion to illustrate how to implement dynamical systems models. It should be kept in mind however, that numerous other models could also be utilized in the same manner. In the following paragraphs the damped linear oscillator model will be introduced via a physical example, linear equations will be given that govern the model, and equivalent differential equations will be shown.

Damped Linear Oscillator

Let us consider a pendulum swinging back and forth on a table. In order to fully explain the action of this system, three pieces of information are required. The first necessary piece of information is the **position** of the tip of the swinging pendulum. The next piece of information needed is the **velocity** of the pendulum. Velocity is the speed of the pendulum, but it takes into account direction as well. For example, if the pendulum is swinging to the right its velocity would be positive and to the left it would be negative (or vice versa). The last piece of information needed to fully model the system is the **acceleration** of the pendulum. Acceleration measures the change in velocity of the pendulum, such that if the pendulum is speeding up acceleration is positive and if it is slowing down acceleration is negative. With these three pieces of information it is possible to completely describe the action of this physical system at a given moment in time.

Once these three necessary pieces of information have been gathered, it becomes a matter of combining them mathematically in a manner that makes them interpretable. The pendulum has been studied extensively by physicists, and although this system may seem like a fairly new idea in the social sciences, it has been well understood for decades in other disciplines. Borrowing from their knowledge, it is known that the following linear equation governs the system of an oscillating pendulum:

$$\frac{d^2x}{dt^2} = \eta\, x + \zeta\, \frac{dx}{dt} \tag{1}$$

where x is the position of the pendulum, dx/dt is the velocity of the pendulum, d^2x/dt^2 is the acceleration of the pendulum, and eta, η, and zeta, ζ, are linear regression coefficients (Hubbard & West, 1991). This equation is a multiple regression equation. Acceleration is the dependent variable, while position and velocity serve as linear predictors. There are two parameters in the model, the coefficients for the linear predictors (eta and zeta). Eta gives a measure related to frequency, or how fast the pendulum swings back and forth. Although the estimated values for eta obtained through fitting this model are difficult to interpret directly, through the use of the following formula an interpretable metric can be obtained:

$$\omega = \frac{1}{2\pi\Delta t}\sqrt{-\eta} \tag{2}$$

where omega, ω, is a measure of frequency in oscillations per unit time and Δt is the distance between two consecutive time points. Zeta gives a measure of *damping*, or how much the magnitude of the amplitude of a cycle changes over time. One can think of this in terms of friction gradually reducing how far the pendulum swings in each cycle with the pendulum eventually coming to rest (Serway & Jewett, 2009).

The system of a single swinging pendulum is not a system of interest to modern researchers, however there are many systems that have similar characteristics to that of an oscillating pendulum and can be modeled using the same ideology. The key idea in applying this model to other systems is to look at the relationships between position, velocity, and acceleration. Let's think of position, x, as the current value of some variable at time, t. We can then think of velocity, dx/dt, as how fast x is changing per a given unit of time (i.e. the speed of a car tells you how fast your moving, which is a change in position). Likewise, we can think of acceleration, d^2x/dt^2, as how fast our velocity, dx/dt, is changing per a given unit of time (i.e. the acceleration of your car tells you how fast you are speeding up, which is a change in velocity). Thinking of the variables as measuring change in each other allows for researchers to move beyond the system of a pendulum and apply the same ideology to other systems that may be of more substantive interest.

Mathematically, the rate at which a value is changing is often explained using the slope of a line. Because the slope measures the change in vertical position (change in position, x, in Figure 1) per change in horizontal position (change in time in Figure 1), it makes sense to model rates of change this way. In calculus the slope of a line is called the first derivative and is often denoted dx/dt. Looking back to Equation 1, this shows that the variable associated with zeta, ζ, in the regression equation is measuring the slope of the measured variable, x, or the first derivative. An equation in which derivatives are used as predictors is known as a *differential equation*.

Since acceleration is also a measure of how fast something is changing (i.e., change in velocity), the same mathematical concepts can be applied. If instead of plotting position against time, as in Figure 1, velocity was plotted against time, the instantaneous slope would give the acceleration, as in Figure 2. It is important to notice however, that in plotting velocity instead of position on the Y-axis in Figure 2, the slope is measuring a change in a different variable. Instead of measuring change in the measured variable in Equation 1, x, it now denotes a change in the first derivative, dx/dt. This means that the slopes in Figure 2 cannot be directly used in the linear regression of Equation 1. This issue can be resolved though by looking at the relationship between the plots in Figures 1 and 2.

Acceleration, as measured as a slope in Figure 2, for two consecutive time points is the difference in velocity for those two time points. This can be measured in Figure 1 by finding the two slopes that represent the two velocities and taking their difference. One could think of this as measuring the change in two rates of change, or slopes. Since acceleration is two measures of change removed from position, in calculus it is called the second derivative and denoted d^2x/dt^2. By calculating acceleration this way, the original metric of position is maintained allowing for acceleration to be used in the regression in Equation 1. One can see that the second derivative, d^2x/dt^2, of the measured variable, x, is the dependent variable in Equation 1.

In many physical systems the application of this differential equation model is extremely straightforward, since the position, velocity, and acceleration of the system are all readily observable or easily estimated through frequent measurement and/or the use of instruments. For systems in the social sciences however, often the variable being measured (analogous to position for a pendulum) is the only available data. Without the ability to measure the first and second derivatives of the variable of interest, in order to fit these models it is necessary to then estimate these values. Several methods have been developed to accomplish this for the types of data sets commonly found in the social sciences (relatively small data sets with large amounts of noise; Boker & Nesselroade, 2002; Boker, Neale, & Rausch, 2004; Deboeck, 2010). For the purposes of this discussion, only the method of Latent Differential Equations (LDE; Boker et al., 2004) will be examined.

As with all statistical models, some assumptions must first be made in order for the models discussed throughout the rest of this paper to be fully understood or fit to data in any interpretable way. For the dynamical systems models of interest here, there are two key assumptions that need to be made that merit mentioning. The first is that the same intrinsic dynamics fit every individual in the data. This does not mean that each individual gets exactly the same model, but merely that the structural paths are the same for all participants. This is a common assumption to structural equation modeling and is not a major limitation of the applicability of these models. Furthermore, this assumption can be relaxed using a random coefficients modeling approach, which would allow for varying parameters across individuals (Boker & Nesselroade, 2000). The second major assumption is that the dynamics of the system remain constant over time. Since it is very difficult to know whether the dynamics of a system have changed in many settings, this assumption may be problematic. Through the use of multilevel methods however, this assumption can also be relaxed to allow parameters to vary over time in cases where the assumptions seems unlikely (Molenaar, Hofer, & Alwin, 2008).

Latent Differential Equations Method

The LDE method uses the framework of SEM to estimate the necessary derivatives in fitting the damped linear oscillator model. The SEM model for this method is similar in structure to a latent growth curve (see Figure 3). The latent variables represent the derivatives in the model, so the paths between the latent variables are the paths of interest in estimating the eta and zeta parameters of Equation 1. The key to fitting this model is to fix the loadings of the latent variables on the observed variables in such a way that the latent variables capture the information of the derivatives they are designed to represent.

In order to fix the loadings in such a way that they accurately estimate the necessary derivatives, the data must first be restructured by a method known as *embedding* (Takens, 1981). Embedding is a process that partitions a set of time points into multiple, shorter sets of time points, and then uses all of those shorter sets of data to create a matrix. This process is similar to many of the "moving window" procedures common in statistics. Each row of the embedded matrix represents one "window", or more importantly one set of manifest variables, that can be used to fit the model. Each row is used as manifest variables to separately estimate the LDE model, and then the separate estimates are averaged to calculate the respective eta and zeta estimates for the full set of time points. This is similar to using separate individuals' observations to calculate group parameters in growth curve modeling.

In order to create an embedded matrix, two values must be selected. The first value is the *embedding dimension*. The embedding dimension indicates the length of each row of the embedded matrix, and thusly the number of manifest variables in the model. Selecting the optimal embedding dimension for a given system is often difficult (Boker & Nesselroade, 2002), and situationally dependent on the data. The second value that must be selected is the *lag*. The lag indicates the distance between two consecutive time points in each set. For example, a lag of one means consecutive time points are selected, a lag of two means one time point is skipped between time points in each short set, etc. In situations with very frequently sampled, noisy data, a lag greater than one can help the researcher avoid some of the possible issues created by the random error, and thusly better capture the dynamics of interest. Selecting the most appropriate lag for a given system is a problem that has been thoroughly discussed in the literature (Deboeck, Boker, & Bergeman, 2008). An example embedded matrix for a data set with n time points, an embedding dimension of five, and a lag of one is seen in Equation 3.

$$\begin{bmatrix} x_1 & x_2 & x_3 & x_4 & x_5 \\ x_2 & x_3 & x_4 & x_5 & x_6 \\ x_3 & x_4 & x_5 & x_6 & x_7 \\ \vdots & \cdots & \cdots & \cdots & \vdots \\ \vdots & \ddots & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ \vdots & \cdots & \cdots & \cdots & \vdots \\ x_{n-4} & x_{n-3} & x_{n-2} & x_{n-1} & x_n \end{bmatrix} \tag{3}$$

Once the data has been correctly embedded, the loadings between the latent and observed variables can be calculated. A generalized way to calculate the values at which to fix the loadings has been developed for the LDE model (Boker et al., 2004). Take one set of indicators from the embedded matrix as a given window in time (e.g. x_1, x_2, x_3, x_4, x_5). For that window, set the midpoint of the window (e.g. x_3). If t is the distance in time between each observation and the midpoint and i is the order of the derivative that the loading goes to, then the following equation can be used to calculate the loading between any given indicator and latent variable,

$$\lambda_{ti} = \frac{(t)^i}{!i} \tag{4}$$

Using Equation 4, the loadings for any number of indicators and latent variables can be computed, which adds flexibility to the possible models that can be implemented. The matrix of factor loadings for the model presented in Figure 3 is

$$\begin{bmatrix} \mathbf{1} & \mathbf{-2t} & \mathbf{2t^2} \\ \mathbf{1} & \mathbf{-1t} & \mathbf{0.5t^2} \\ \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{1} & \mathbf{1t} & \mathbf{0.5t^2} \\ \mathbf{1} & \mathbf{2t} & \mathbf{2t^2} \end{bmatrix}. \tag{5}$$

A drawback of fitting the model in Figure 3 using the LDE method, as well as many other methods for fitting the damped linear oscillator model, is that only the oscillating trend can be present in the data. Any over-arching linear (or other trend) that may also be present in the data must be somehow removed from the data prior to fitting this model. Since these other trends are often of just as much interest to the researcher as the oscillation, this is a deterrent to implementing these methods. Currently, two-step procedures are used, where first any trend is removed, and then the residuals from that step are used to fit the model (Bisconti et al., 2006). Not only is this additional work for the researcher, but it also does not employ simultaneous estimation which can affect parameter estimates and their standard errors (Maxwell & Delaney, 2004). The current study introduces a method that allows for the trend and damped linear oscillator model to be estimated in one step with simultaneous estimation.

The Higher-Order Derivative Method

The current method uses higher-order derivatives and some common SEM ideas to allow simultaneous estimation of trends at the same time as the damped linear oscillator model. The main idea that powers this method is that the relationships captured in Equation 1 that govern the damped linear oscillator model are maintained regardless of the order of the derivatives used, so long as the relative distance between the orders of the derivatives is consistent (Chow, Ram, Boker, Fujita, & Clore, 2005). For example, Equation 1 shows the zeroth, first, and second order derivatives, but if they were substituted for the fourth, fifth, and sixth order derivatives, respectively, the values and interpretations of eta and zeta would not change. This is because the eta and zeta coefficients capture information about the relationships among the three derivatives, which as will be shown, do not change across increasing derivative orders.

It was previously discussed that the first derivative measures the rate of change in the zeroth order derivative. Graphically, this was illustrated by showing that a slope (i.e., the first derivative) is a measure of the rate of change in the variable of interest (i.e., the zeroth order derivative). Likewise, the second order derivative is a measure of rate of change in the first order derivative, as can be seen through the example of finding acceleration (i.e., the second order derivative) as the difference between two velocities, or slopes, or first derivatives. Thusly, the relationship between the zeroth and first derivatives and first and second derivatives is essentially the same, one is a measure of rate of change of the other. It can be shown that this relationship holds for all orders of consecutive derivatives, so long as the system can be continuously differentiated (Stewart, 2011). From this idea, it follows that the relationship between derivatives two orders apart (i.e., the zeroth and second order derivatives) would also be the same regardless of the absolute orders involved. From this, it stands to reason that since eta and zeta are measures of the relationships between derivatives, they too will be unaffected by the absolute order of the derivatives in the model, so long as the relative distance between the derivatives remains the same.

In order to illustrate how this idea allows for simultaneous estimation of over-arching trends and the damped linear oscillator model, the problem created by the presence of a trend for these models must be more thoroughly examined. Consider Figure 4 which depicts two damped linear oscillator models, one with and one without a positive, linear trend. The presence of the linear trend alters the values of the zeroth order derivative, which is visible in Figures 4a and 4e. The first order derivative is also changed by each value increasing by the over-arching trend's slope as can be seen in Figures 4b and 4f. The second and third order derivatives (Figures 4c and 4g and Figures 4d and 4h, respectively) are not affected by the linear trend though. These changes in the derivatives alter how they relate to each other as well, and thusly impacts the estimates obtained in the LDE model.

Figure 4 demonstrates that the impact of adding a linear trend to the DLO model only the changes relationships involving the zeroth order derivative. The second and third order derivatives are unaffected. The first order derivative was uniformly increased by the slope of the trend, which alters its values, but it's relationships with the other derivatives are unaffected. This means that the relationships among the first, second, and third order derivatives are maintained even with the addition of the over-arching linear trend. It has already been discussed that any three consecutive derivatives can be used to estimate the LDE model. Thusly, even with an over-arching linear trend the first, second, and third order derivatives can be used to estimate the eta and zeta parameters in the LDE model.

Methods

Simulation Design

A simulation was conducted to analyze the accuracy of the proposed method for estimating certain model parameters, as well as to compare its performance to the existing, two-step LDE method. Both the higher-order derivative model and the corresponding LDE model were fit to the same data. The time metric and amplitude of the data were rescaled by factors of 0.02 and 10, respectively, for the higher-order derivative models to avoid computational precision issues in the software, and this alteration to the data was retained for the LDE models to maintain data consistency. R version 2.15.0 (R Development Core Team, 2012) was used with the "OpenMX" (Boker, Neale, Maes, Wilde, Spiegel, Brick, & Fox, 2011; B oker, Neale, Maes, Wilde, Spiegel, Brick, & Fox, 2010) and "odesolve" (Setzer, 2005) packages to simulate the data for each condition and fit the appropriate models. Path diagrams for both models can be found in Figures 5a and 5b. An embedding dimension of five and a lag of one were selected for the models. These two values were chosen because, in conjunction with the range of eta and signal-to-noise parameters chosen, they would give identified models that span the range of models found to accurately recover eta and zeta based upon previous studies (Boker et al., 2004). The covariances between the zeroth derivative and all other derivatives in the higher-order derivative model were fixed to zero. This fix was done to identify the model, and since these three parameters were of little interest to the current study. The fixed value of zero was chosen based upon results obtained by the researchers in preliminary tests. In conditions with an over-arching trend equal to zero, the structural paths between the zeroth, first, and second derivatives could be estimated (same as the LDE model), but to maintain consistency the parameters were fixed for every condition. In order to fit the two-step LDE model, the over-arching trend in the data was removed by fitting a linear model to the data (Step 1), and then the LDE model was fit to the resulting residuals (Step 2), as is the norm for the two-step approach.

Simulation Conditions

One hundred equally-spaced observations composed each simulated time series. Four parameters were varied in the simulation. Five eta values were used {-0.5, -0.4, -0.3, -0.2,-0.1}[1]. These five values span the range of eta values across which the LDE method has been found to be effective (Boker et al., 2004). Five values of zeta were examined {-0.05, -0.025, 0.0, 0.025, 0.05}. Six different over-arching linear slopes were used {0.0, 0.025, 0.050, 0.075, 0.1, 0.2}. All over-arching slopes tested were positive, as negative slopes would behave in the same way. Three *signal-to-noise ratios* were also tested {20:1, 5:1, 2:1}. The signal-to-noise ratio is a ratio of the variance produced by the model to random error variance. For example, a signal-to-noise ratio of 10:1 would indicate that the variance of the model dynamics, or signal, is ten times greater than the error variance, or noise. These ratios were calculated in reference to only the variance of the DLO model (variance introduced by the over-arching trend was not included), against some proportion of induced random variance. The values of each parameter were crossed (i.e., a 5x5x6x3 design) to create 450 total simulation conditions. 1000 time series were analyzed for each condition, resulting in a total of 450,000 time series each analyzed using both the higher-order derivative and two-step LDE methods.

Results

Two separate questions need to be addressed in looking at the simulation results for this study. First, the effectiveness of the higher-order derivative method must be examined in terms of how well parameters are estimated under each condition. Since the eta, zeta, and trend parameters are often of most interest in studies that employ the DLO model, these three parameters will be examined to establish how much bias is present using the higher-order derivative method. Second, it must be shown if the higher-order derivative method performs as well as, or better than, the two-step LDE method, and if so under what conditions.

Model Convergence

Only parameter estimates from iterations that converged to a solution were used to calculate the overall condition parameters for the higher-order derivative method (Gill, Murray, Saunders, & Wright, 1984). Conditions with numerous, non-converging iterations likely represent situations in which the model fit to the data cannot reliably produce trustworthy parameter estimates. These conditions are thusly not included in the calculations in subsequent sections determining the effectiveness of this method in estimating the parameters of interest. A threshold of seventy-five non-converging iterations (7.5%) was set by the researcher to assess whether a condition would be included. Convergence for the LDE method was examined, but in order to best compare the comparative effectiveness of the two estimation methods, only the conditions for which the higher-order derivative approach converged were used in the comparisons of parameter estimation accuracy. Figure 6 shows a graph indicating the general distribution of non-convergence for both the higher-order and LDE methods. The higher-order derivative method met the threshold for convergence much more often (60.2%) than the traditional, two-step LDE approach (2.4%).

The four manipulated factors in the simulation were examined to see if they had any effect on whether the higher-order derivative method met the threshold for convergence (Table 1). The values of the true eta and zeta parameters had minimal impact on the number of converging conditions. As the over-arching trend increased (steeper slope), the number of converging cases decreased. Also, as the signal-to-noise ratio increased (less noisy data), the number of converging cases increased.

It is important to note that removing the simulation conditions that do not meet the threshold for convergence from the analyses that assess the accuracy of the two estimation methods, can make drawing inference from analyses more difficult. Because many simulation conditions were not used in assessing the bias and efficiency of these methods (39.8%), the levels of the manipulated factors in the simulation no longer had an equal number of cases. This potentially complicates drawing conclusions from the results, since differing sample sizes can alter how one sees the data. To see an example of this, consider the hypothetical situation for some study with a parameter of interest, lambda (λ), shown in Figure 7. Looking only at the number of conditions (Figure 7a), one would find an obvious effect of true λ on whether a given method is more accurate than another. However, if you take into account the number of cases that converged at a given level of λ and look at the percentage of possible conditions (Figure 7b), one could infer that the true λ of the condition had little, if any, effect. In order to avoid this potential problem, some of the results presented in this study were not only analyzed in terms of the number of cases, but also as percentages based on the number of converging conditions.

Eta

The higher-order derivative method estimated eta well under certain conditions (see Table 2). Extreme values of eta were found under most conditions, and thusly mean values of eta were found to be significantly biased, so median eta values were used to try to reduce the effect of these extreme values and measure the method's effectiveness in estimating eta. By looking at the mean squared error (MSE) between the median and true eta values, as well as correlations between the percent bias and the manipulated factors for each simulation condition, several patterns emerge illustrating under what types of situations this method could accurately recover eta. The steepness of the over-arching trend was the most influential factor in recovering eta with a correlation of 0.509. As the over-arching trend's slope increases in magnitude, the MSE of eta increases. The true value of eta also impacted the effectiveness of this method in estimating eta having a correlation of 0.385 in magnitude. As the value of the true eta value decreases in magnitude, the MSE of eta increases. It should be noted that the value of zeta had little to no effect on estimating eta.

Median estimated eta values were also used to compare the two estimation methods in order to reduce the effect of extreme values estimated by either method. The higher-order derivative approach produced a more accurate median eta estimate, using the absolute value of the error in the medians as the measure of accuracy, in 90 of the 271 (33.0%) converging conditions. The higher-order derivative method (mean error of 0.835 and a total error of 226.3) produced much smaller errors overall than LDE (mean error of 6.200 and a total error of 1680.1) (See Figure 8).

Figure 9 shows the frequencies of the four manipulated variables in the simulation for the conditions that the higher-order derivative method was more accurate than the LDE approach.

The manipulated simulation factors of true eta, zeta, and over-arching trend, all showed effects on which method was more accurate in estimating eta whether the number of converging conditions at each level of the variables was taken into account or not. The higher-order derivative method performed better than the two-step approach more often for longer cycles (etas with larger magnitude) with 60 of the 90 conditions having a true eta of -0.5 or -0.4. The higher-order derivative method yielded more accurate eta estimates than LDE for conditions with zeta greater than zero with 69 of the 90 cases (76.7%) having positive zeta parameters. The over-arching trend had minimal effect on whether the higher-order derivative method produced better estimates than the LDE approach. The impact of signal-to-noise ratio was ambiguous depending on whether the number of converging conditions at each level was considered. The higher-order derivative method outperformed LDE more often for cases with smaller signal-to-noise ratios (more noise in the data) with 73 of the 90 conditions (81.1%) having signal-to-noise ratios of 2:1 or 5:1. However in terms of the percentage of possible conditions, no effect was found.

The LDE approach produced more accurate eta estimates in a wider range of conditions than the higher-order derivative method (67.0‰) as can be seen in Table 3. For conditions with longer cycles (lesser etas), the two-step approach was better. The LDE method was significantly more accurate in conditions with signal-to-noise ratios of 2:1, and marginally more accurate in cases with a ratio of 5:1, suggesting that the two-step approach is less negatively impacted by noise. The LDE method also is more accurate in recovering eta for conditions with decreasing amplitudes (zeta less than zero).

Zeta

The higher-order derivative method had the most biased estimates in recovering the zeta parameter; however, under certain simulation conditions zeta was accurately estimated. Extreme values were found to be estimated under many simulation conditions, so median zeta values were used instead of means to assess the accuracy of the method in recovering zeta, since medians are relatively unaffected by extreme values compared to means.. The manipulated factors eta, trend, and signal-to-noise ratio were found to have no significant effect on how accurately the zeta parameter was recovered using the higher-order derivative method based upon their low correlations with the percent bias in zeta estimates (all were less than 0.2 in magnitude). The true zeta value had a positive correlation of 0.364, suggesting a moderate association. This would suggest that as zeta increases, the ability of the higher-order derivative method to accurately recover it decreases.

The LDE method also had the most difficulty in accurately recovering the zeta parameter compared to eta and the over-arching trend. Using the absolute value of the error of the median zeta estimates as the measure of accuracy, to avoid the impact of extreme values on the analyses, of the 271 converging conditions the higher-order derivative method had a more accurate zeta estimate in 129 of them (47.6%). Although the two estimation methods were basically equal in the number of conditions for which they more accurately recovered zeta, the higher-order derivative method (mean error of 0.165 and a total error of 44.7) produced much smaller errors than the LDE approach (mean error of 5.504 and a total error of 1491.5) (Figure 10).

The true eta of the simulation condition had little to no effect on whether the higher-order derivative produced a more accurate zeta estimate than LDE. Over the range of etas tested the percentage of conditions for which the higher-order derivative method was less biased was always between 45% and 53%. The true zeta had a well-defined effect as to which method was more accurate in recovering zeta. For true zetas greater than zero, the higher-order derivative method was more accurate than LDE in 82.1% of cases, while only more accurate in 21.4% of the simulation conditions with a true zeta less than or equal to zero. The effects of the conditions' true over-arching trend and signal-to-noise ratio on determining which method was more accurate was less clear. In terms of the number of conditions, as both the over-arching trend and signal-to-noise ratio decreased (less steep trend and less noise in the data), the higher-order derivative approach outperformed LDE more often. However, if the number of converging conditions at each level of trend and signal-to-noise ratio are taken into account, both factors show no effect on whether the higher-order derivative method is more accurate. Given the results the two-step approach is best used to recover zeta if it is not positive, and the higher-order derivative method is best if it is.

Trend

For the higher-order derivative method the over-arching trend was well recovered for all of the conditions that converged. All of the estimated mean trends had a percent bias of 5% or less, with 218 of the 271 conditions (80.4%) having a percent bias of less than 1%. Since all converging conditions accurately estimated the over-arching trend using this method, the researchers did not examine the effects of the other factors on trend estimation as no effect would be significant.

The LDE method recovered a more accurate trend estimate than the higher-order derivative method in nearly all of the converging conditions, using the absolute error in the median trend estimates as the measure of accuracy. Since the higher-order derivative method produced such accurate trend estimates though, the improvement in the true trend estimates between the two methods is minimal. With both estimation procedures recovering accurate estimates of the over-arching trend, and the LDE method being more accurate in all conditions, the effects of the manipulated simulation factors on the median estimates were not examined since all four effects would be negligible. Although the two-step LDE approach produced slightly less biased estimates of the trend parameter (mean gain in bias of 0.000459 and a total gain in bias of 0.125), the higher-order derivative method produced more precise estimates (mean gain in standard errors of 0.0400 and a total gain in standard errors of 10.841) compared to the two-step LDE approach, as measured by standard errors, in 270 of the 271 conditions (99.6%).

Discussion

Conclusions

The higher-order derivative method provides an improvement over the existing, two-step, LDE approach under certain conditions based on the results in this study. In situations with longer, more heavily sampled cycles (etas with larger magnitude), a growing amplitude (zeta greater than zero), and a relatively small over-arching trend (flatter slope), the higher-order derivative approach is more accurate in recovering eta and zeta. In nearly every condition however, the proposed method yields more precise estimates of the over-arching trend, which is to be expected when going from a two-step method to a one-step method with simultaneous estimation. Although the LDE approach does produce slightly less biased estimates of trend , which is to be expected since the two-step approach produces unbiased estimates, the gain in precision from using the higher-order derivative method was always greater than the difference in bias for the two methods, showing that more precision is gained than accuracy is lost in estimating trend using the higher-order derivative method.

The accuracy in the median estimates of the three parameters of interest (eta, zeta, and trend) was better in magnitude overall for the higher-order derivative approach than LDE, but the two-step approach was more accurate over more conditions. The higher-order derivative method produced much smaller total absolute errors when estimating eta and zeta than LDE. The LDE method did recover more accurate trend estimates, but both methods were very accurate so the improvement is negligible in most situations. The improvement in overall accuracy for the parameters of interest suggests that when a higher-order derivative model produces poor estimates, the gain in bias is less than that of the two-step LDE model on average. Although not producing poor estimates is always preferred, in situations in which the researcher may be unsure of whether estimates are poor, the higher-order derivative method is often a safer choice than the LDE approach since it produces smaller gains in bias.

There are still many situations in which the two-step LDE approach produces more accurate estimates than the higher-order derivative method, and is thusly a better model. For very steep over-arching trends relative to the amplitude of oscillation (trends of 0.2 in this study), the two-step approach produced much more accurate estimates of eta and zeta. It is possible that the large trend “washes out” the dynamics created by eta and zeta in the simultaneous estimation of the higher-order derivative method, but this issue is avoided by first removing the over-arching trend in the two-step approach. Noise has less of a detrimental effect on the two-step LDE approach. In situations with noisy data (signal-to-noise ratio of 2:1 in this study) the LDE approach produced much more accurate eta and zeta estimates, thusly making it the better model. This is to be expected since the effects of random error are amplified as the order of the derivatives in the model increases. The LDE method also performed better in terms of accurately recovering eta for cycles that are long relative to the time interval spanned by one set of indicators (etas of -0.2 and -0.1 in this study).

Taking all of the above information into account, whether or not the proposed, higher-order derivative method or the traditional, two-step LDE approach is best depends on the particular data being modeled. In many cases, theory or previous studies can give an indication as to likely values for parameters. For example, females ovulate monthly (a monthly cycle) so using that information one could get a good idea of the expected eta values (see Equation 2) based on any sampling interval. In situations where the researcher has no way of knowing likely values for the parameters of interest prior to the study, the author recommends running both models on a randomly selected subset of the data (33.3%), and then using those results to decide which approach is the most appropriate.

Weaknesses and Future Considerations

The large number of non-converging iterations, especially for the LDE model, is a major limitation of this study. Some of the non-convergence was expected based upon the chosen values for the manipulated factors in the simulation, as the researchers wanted to find a range of working parameters. Results obtained in a previous study (Boker et al., 2004) mention that if (a) the interval of time spanned by one set of indicators is greater than one half the time interval of an oscillation cycle and/or (b) the communalities among indicators are very low, then models such as those used here may not converge, but do not report how often. These two conditions also cause bias to increase rapidly, which may explain the large MSE values found for eta and zeta, especially for the higher-order derivative method, for conditions with large signal-to-noise ratios. The true eta value of -0.5 produces conditions that create a sampling interval longer than one half the length of a cycle, which could explain non-convergence for those cases. The necessary rescaling of time due to software precision issues produced some conditions with small factor loadings, and thusly small communalities, relative to the amount of random error.

This is another possible explanation for some of the non-converging cases. As this study introduces trend directly to the SEM model for the first time, it is difficult to assess how the over-arching trend is affecting convergence. Based on the results obtained here, it seems that as the trend gets steeper convergence decreases. There is even some evidence of a threshold value for trend, at which model convergence drops significantly. Future simulations should attempt to correct these areas in order to possibly improve convergence rates.

The decision to use the same cases that converged for the higher-order derivative method and the LDE approach in comparing the two estimation procedures, regardless of whether the LDE method reached the threshold for convergence for those conditions, is also a limitation of this study, but it was deemed reasonable for several reasons. The first reason is that the LDE method has been found to produce trustworthy parameter estimate across a wide range of conditions (including those used in this study) in previous literature (Boker et al., 2004). Secondly, the researchers constructed a correlation table between the number of non-converging iterations and the three parameters of interest in this study and found no correlation with magnitude greater than 0.08. Additionally, to verify the LDE parameter estimates obtained, a random subset of conditions were selected and re-analyzed using the lavaan package in R (Rosseel, Oberski, & Byrnes, 2010; Rosseel, 2012). The medians for the three parameters of interest had a high level of agreement for LDE between the two software packages. Given these reasons, the researchers decided that the LDE output was trustworthy to compare the two methods, regardless of the convergence of LDE. The frequent non- convergence of the LDE approach in the OpenMx package is possibly due to complexities in the likelihood space, and this is an area where future studies are needed (Gill, Murray, Saunders & Wright, 1984).

In addition to future studies remedying the above weaknesses, there is more work to be done based upon the results obtained in this study. The effect of missing data, both on the bias of estimates and relative accuracy compared to the LDE approach for the higher-order derivative method, is an area of future research that is important, as missing data impacts nearly every study in which this method would be applied. The effect of adding higher-order over-arching trends (i.e. quadratic, cubic) is another area for future study. The researchers also believe that the application of Bayesian estimation procedures to the proposed method may improve its bias, convergence, precision, and efficiency, and is a direction that should be examined.

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Footnotes

[1] The five eta values selected correspond to frequencies (See Equation 2) of {0.113, 0.101, 0.0872, 0.0712, 0.0503}, respectively.

Tables & Figures

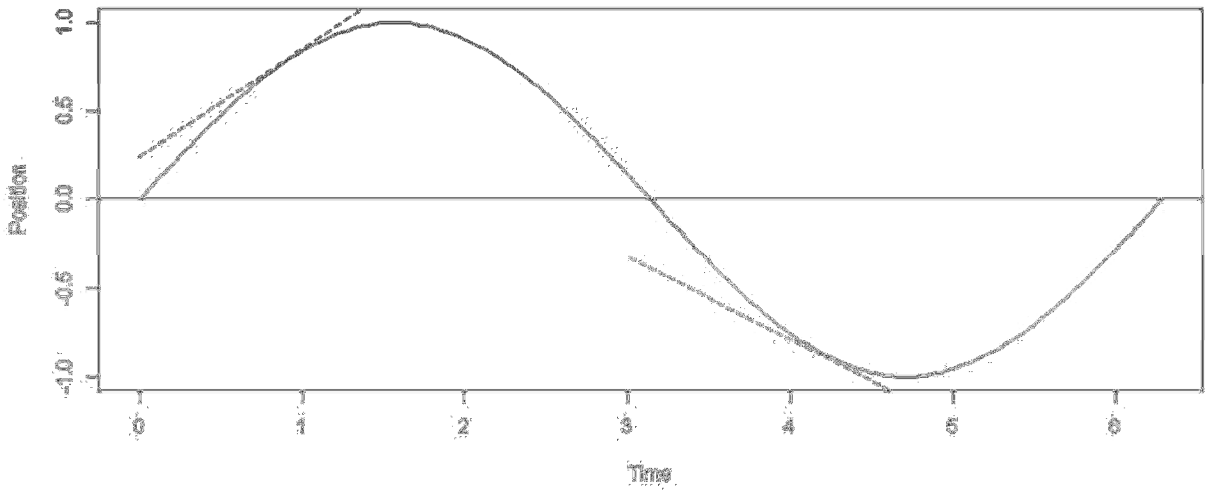

Figure 1. A plot of position versus time for a damped linear oscillator (solid line) with slopes/first derivatives shown (dashed lines).

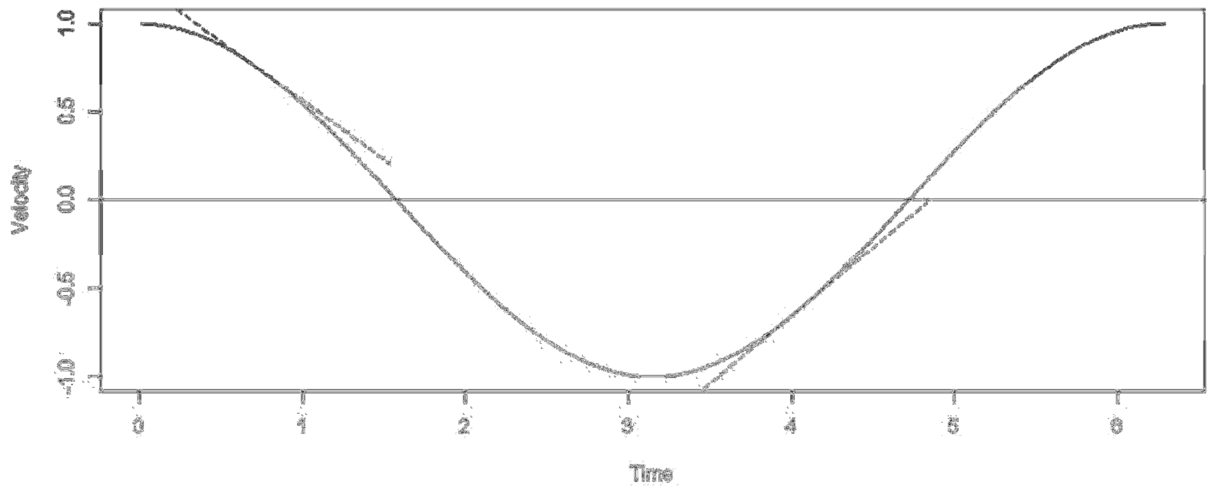

Figure 2. A plot of velocity versus time for a damped linear oscillator (solid line) with slopes/first derivatives, which are second derivatives of x, shown (dashed lines).

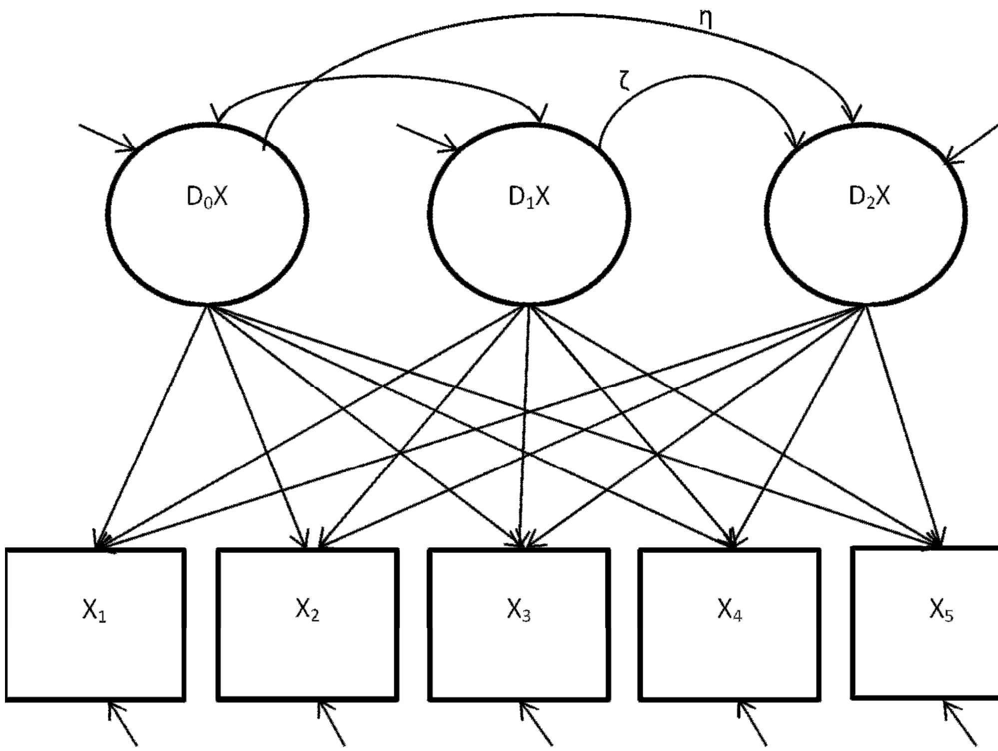

Figure 3. A path diagram of the LDE method of fitting a damped linear oscillator. The latent variables denoted $D_i X$ represent the derivatives with *i* denoting the order of the derivative.

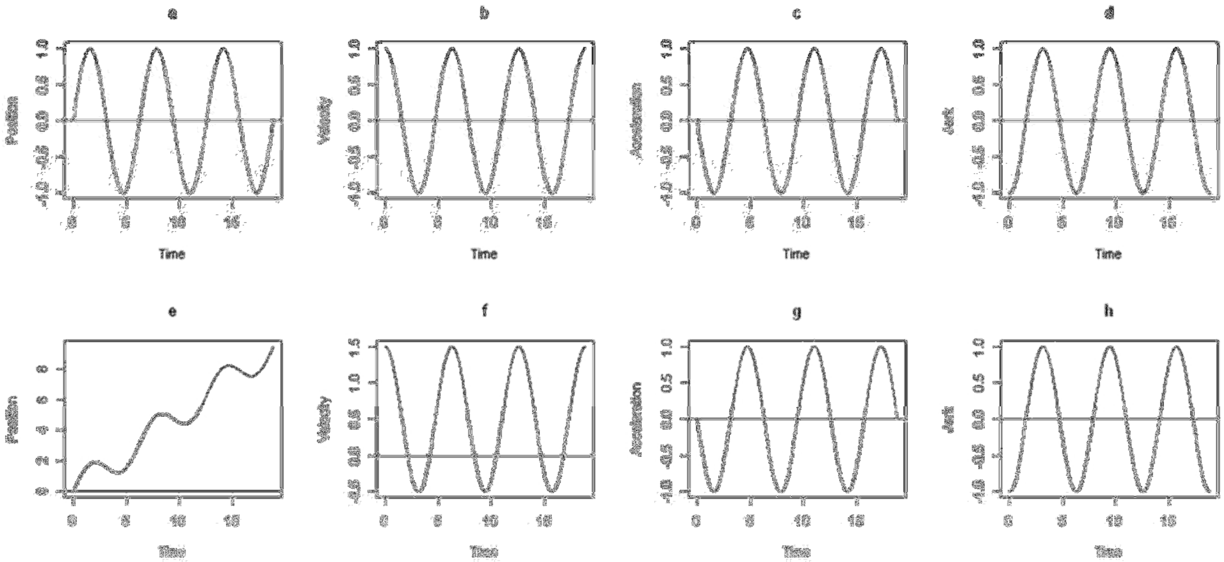

Figure 4. A set of plots for the position, velocity, acceleration, and "jerk" (or zeroth, first, second, and third order derivatives, respectively) for the DLO model. Plots a, b, c, and d are the four plots for a DLO without an over-arching linear trend, and plots e, f, g, and h are the four plots for a DLO with an over-arching linear trend.

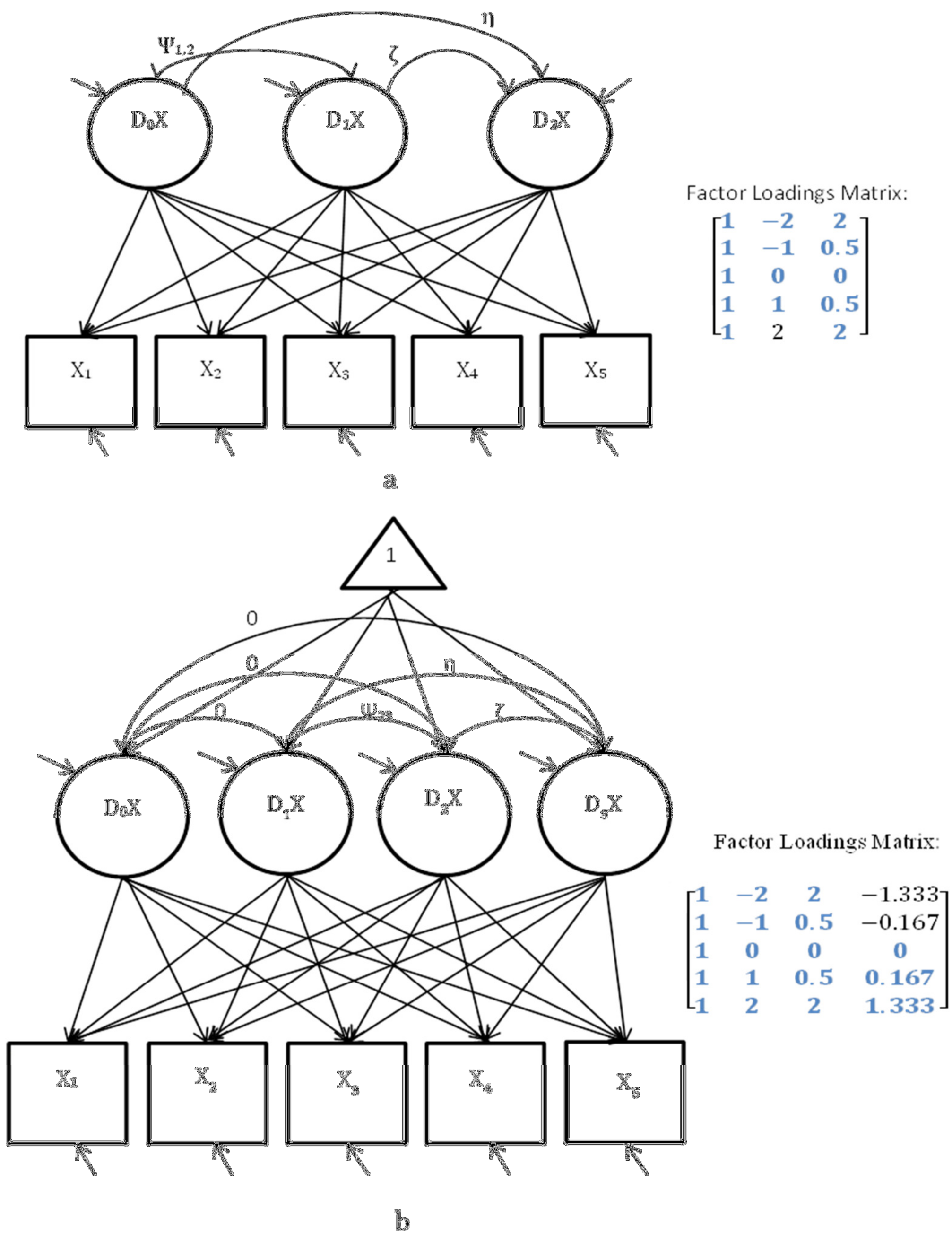

Figure 5. a) The path diagram and loadings matrix for the LDE model. b) The path diagram and loadings matrix for the higher-order derivative model. The four latent means were freely estimated for the higher-order derivative model. All manifest and latent variances were freely estimated for both models. Although the time metric was rescaled in the simulation, which would alter the loadings, this was left out of this Figure for simplicity.

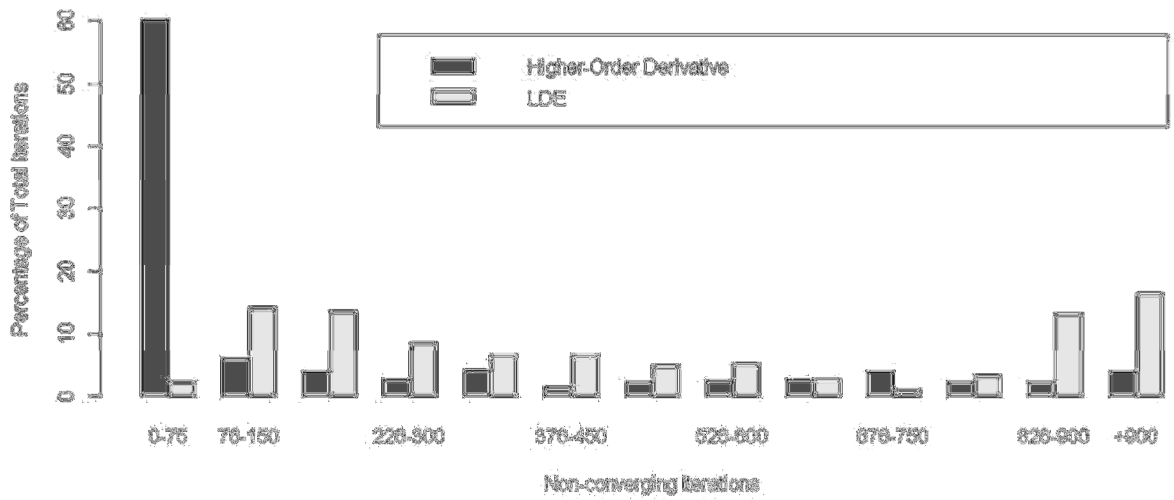

Figure 6. Plot of the percentage of non-converging iterations for both estimation methods.

Convergence Information for Each Manipulated Factor

Eta		Zeta		Trend		Noise	
True η	Count(%)	True ζ	Count(%)	True Trend	Count(%)	Signal-to-Noise Ratio	Count(%)
-0.5	51(56.7%)	-0.05	45(50.0%)	0	62(82.7%)	20:1	130(86.7%)
-0.4	56(62.2%)	-0.025	50(55.6%)	0.025	54(72.0%)	5:1	101(67.3%)
-0.3	48(53.3%)	0	59(65.6%)	0.05	52(69.3%)	2:1	40(26.7%)
-0.2	58(64.4%)	0.025	63((70.0%)	0.075	43(57.3%)		
-0.1	58(64.4%)	0.05	54(60.0%)	0.1	44(58.7%)		
				0.2	16(21.3%)		

Table 1. Table illustrating the number of converging conditions across levels of the four manipulated variables in the simulation for the higher-order derivative method.

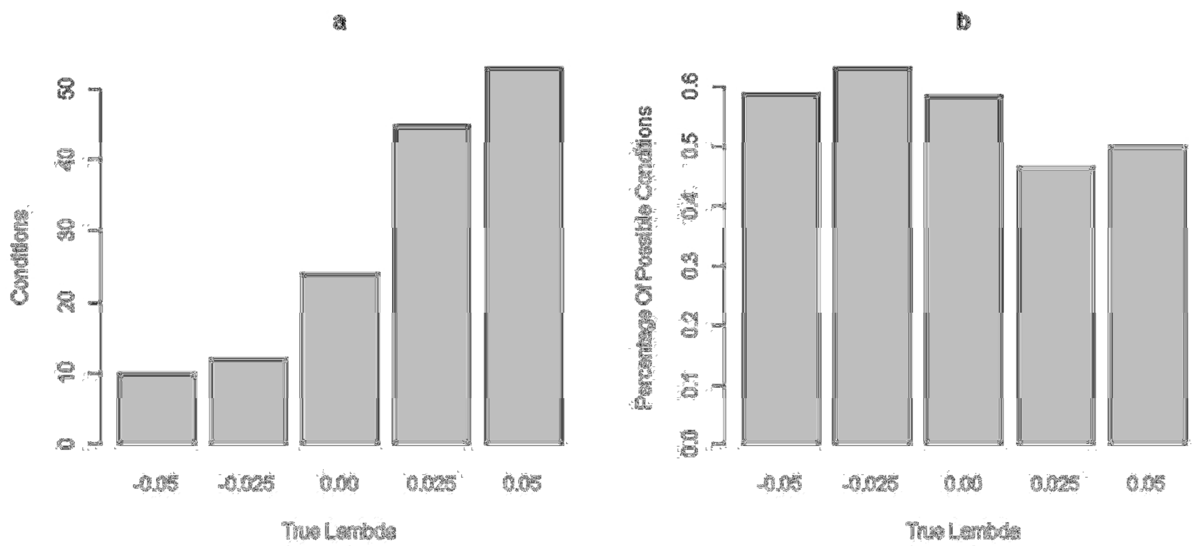

Figure 7. a) Plot depicting the number of conditions for which a given method was more accurate for all values of true λ. b) Plot depicting the percentage of possible conditions taking into account convergence for all values of true λ.

		Noise Ratio of 20:1					Noise Ratio of 5:1					Noise Ratio of 2:1				
Trend	True η	Mean	Median	95% CI		MSE	Mean	Median	95% CI		MSE	Mean	Median	95% CI		MSE
0.000	-0.500	-1.298	-0.485	-8.589	0.000	0.000	-10.623	-1.620	-91.839	0.000	1.311	-2.562	-0.270	-14.812	0.000	3.685
0.025	-0.500	-1.169	-0.426	-4.812	0.000	0.033	-2.678	-0.504	-8.927	0.000	0.050	-4.092	-0.541	-16.653	0.000	0.530
0.050	-0.500	-0.945	-0.814	-2.903	0.000	0.099	-3.908	-1.032	-14.077	0.000	2.360	-6.691	-1.143	-35.725	0.000	3.068
0.075	-0.500	-1.118	-0.512	-4.024	0.000	0.000	-4.743	-0.994	-20.086	0.000	3.759	-3.719	-1.030	-12.458	-0.033	0.459
0.100	-0.500	NA	NA	NA	NA	NA	-4.856	-0.911	-23.355	0.000	0.085	-3.312	-0.649	-11.887	0.000	1.340
0.200	-0.500	NA	NA	NA	NA	NA	-44.957	-3.502	-219.872	0.000	9.013	-33.743	-3.134	-156.949	0.000	9.013
0.000	-0.400	-0.510	-0.394	-0.541	-0.079	0.000	-0.633	-0.397	-1.006	-0.175	0.168	-2.810	-0.377	-14.965	0.000	0.209
0.025	-0.400	-2.809	-0.583	-8.832	-0.002	0.017	-3.212	-0.440	-15.302	0.000	0.346	-6.642	-0.971	-32.469	0.000	0.409
0.050	-0.400	-7.052	-2.628	-26.001	0.000	4.963	-2.696	-0.919	-13.320	0.000	1.137	-4.082	-1.098	-19.343	0.000	2.738
0.075	-0.400	NA	NA	NA	NA	NA	-2.933	-1.133	-13.183	0.000	5.884	-3.845	-0.806	-19.547	0.000	7.591
0.100	-0.400	-0.703	-0.488	-2.153	0.000	0.008	-2.848	-0.846	-17.140	0.000	4.933	-5.021	-1.010	-24.277	0.000	1.143
0.200	-0.400	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	-36.016	-4.028	-149.366	0.000	13.059
0.000	-0.300	-0.524	-0.318	-1.511	-0.083	0.000	-1.576	-0.365	-7.013	0.000	0.010	-1.148	-0.338	-4.579	0.000	2.512
0.025	-0.300	-0.798	-0.387	-3.544	0.000	0.022	-1.860	-0.379	-6.122	0.000	0.547	-1.735	-0.387	-9.827	0.000	0.785
0.050	-0.300	-1.078	-0.673	-3.648	-0.002	0.139	-1.470	-0.738	-6.777	0.000	0.109	-6.071	-0.993	-29.407	0.000	1.754
0.075	-0.300	-0.791	-0.556	-2.551	0.000	0.065	-1.805	-0.650	-7.532	0.000	0.155	-4.982	-0.844	-25.320	0.000	3.905
0.100	-0.300	NA	NA	NA	NA	NA	-2.277	-0.842	-9.749	0.000	0.180	-1.797	-0.883	-8.393	0.000	4.057
0.200	-0.300	NA	NA	NA	NA	NA	-23.168	-2.755	-46.616	0.000	6.027	-34.851	-2.850	-204.196	0.000	5.786
0.000	-0.200	-0.476	-0.256	-1.407	-0.190	0.003	-0.200	-0.191	-0.239	-0.163	0.260	-0.257	-0.218	-0.385	-0.191	1.280
0.025	-0.200	-1.833	-0.381	-7.960	-0.013	0.033	-1.680	-0.544	-8.400	0.000	0.392	-1.272	-0.253	-6.618	0.000	0.694
0.050	-0.200	-2.551	-0.412	-7.357	-0.153	1.900	-3.040	-0.661	-14.620	0.000	0.172	-4.203	-0.870	-21.181	0.000	1.743
0.075	-0.200	NA	NA	NA	NA	NA	-3.858	-0.607	-22.489	0.000	0.125	-3.036	-0.709	-14.410	0.000	1.254
0.100	-0.200	-2.938	-0.408	-8.086	-0.027	0.043	-1.296	-0.514	-5.211	0.000	2.637	-3.308	-0.702	-15.919	0.000	0.988
0.200	-0.200	NA	NA	NA	NA	NA	-24.755	-2.453	-87.367	0.000	4.255	-18.760	-2.431	-62.422	0.000	4.921
0.000	-0.100	-0.321	-0.230	-0.583	-0.105	0.195	-3.112	-0.548	-20.827	0.000	0.325	-8.761	-0.944	-55.023	0.000	1.381
0.025	-0.100	-0.786	-0.223	-4.899	0.000	0.349	-1.392	-0.005	-8.130	0.000	0.996	-1.102	0.000	-6.738	0.000	1.333
0.050	-0.100	-12.179	-0.361	-30.114	0.000	0.271	-3.564	-0.715	-18.054	0.000	0.261	-6.407	-1.314	-29.621	0.000	2.519
0.075	-0.100	NA	NA	NA	NA	NA	-2.230	-0.441	-11.665	0.000	0.585	-6.582	-1.388	-30.832	0.000	1.684
0.100	-0.100	NA	NA	NA	NA	NA	-1.370	-0.408	-6.335	0.000	1.421	-3.098	-0.833	-13.273	0.000	1.685
0.200	-0.100	NA	NA	NA	NA	NA	-17.865	-1.809	-45.501	0.000	2.922	-19.503	-2.472	-72.607	0.000	7.494

Table 2. A table showing eta estimates and other statistical information. Zeta was not a significant factor in estimating eta, so it was averaged over. Cells marked with "NA's" denote conditions for which there were not enough converging iterations to perform analysis.

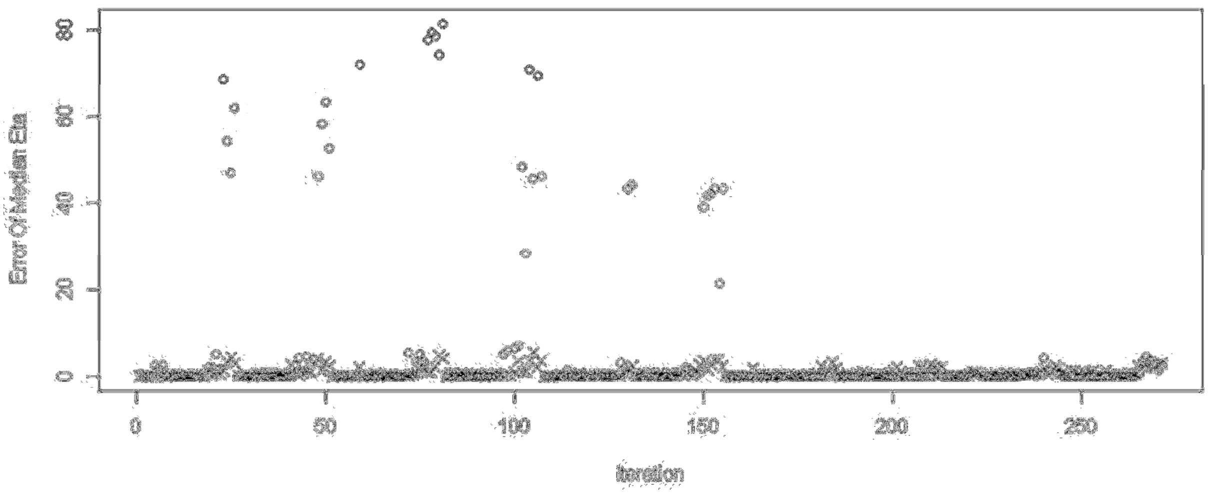

Figure 8. Plot depicting the error of the estimated median etas for both estimation methods. The “X’s” represent the higher-order derivative method, and the “O’s” represent the LDE method. Each converging iteration is shown across the x-axis.

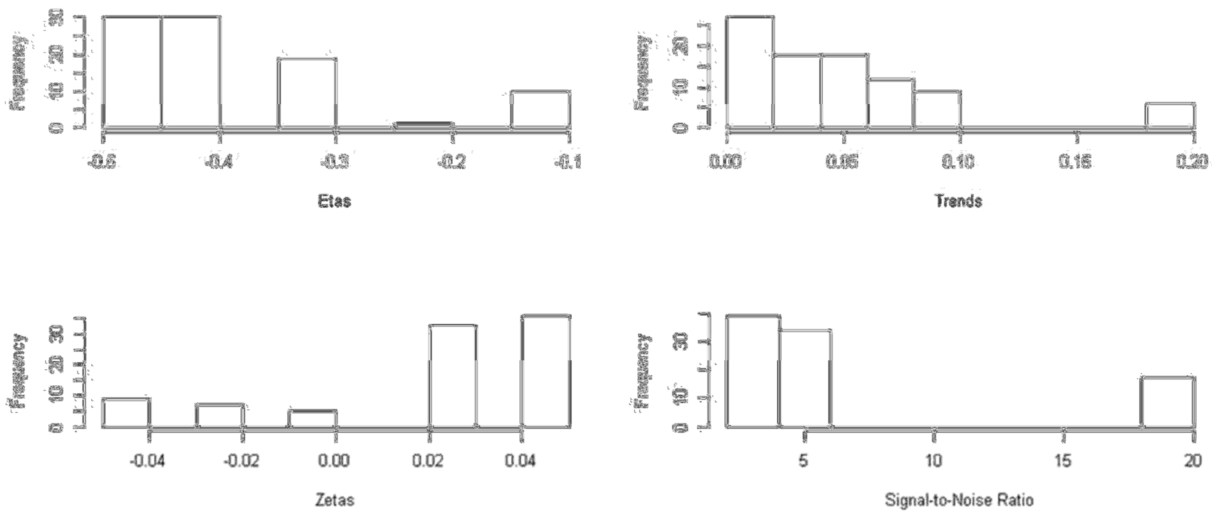

Figure 9. Histograms showing the frequencies of the simulation parameters that were manipulated in the 90 conditions that the higher-order derivative method was more accurate than the LDE approach.

		Noise Ratio of 20:1				Noise Ratio of 5:1				Noise Ratio of 2:1			
True ζ	True η	HO Mean Median	HO MSE	LDE Mean Median	LDE MSE	HO Mean Median	HO MSE	LDE Mean Median	LDE MSE	HO Mean Median	HO MSE	LDE Mean Median	LDE MSE
-0.05	-0.5	-0.485037263	0.00022	-0.070136015	0.18478	-0.860342891	0.17408	-0.424576701	0.00569	-0.622488288	0.08947	-0.426128345	0.00547
-0.025	-0.5	-0.425748275	0.00551	-0.427929727	0.00519	-0.590600179	0.01047	-0.424668075	0.00568	-1.011140008	0.33273	-0.425993001	0.00548
0	-0.5	-0.499756345	0.00015	-0.434927223	0.00423	-0.71625417	0.07069	-0.425203187	0.0056	-7.539715053	-518.38	-0.572312666	0.79332
0.025	-0.5	-0.684184324	0.05339	-2.769991592	5.32405	-1.046317928	0.41647	-3.188531749	9.05512	-9.746455094	-663.66	0	0.25
0.05	-0.5	NA	NA	NA	NA	-3.450364744	9.98016	-58.62456564	3444.96	-3.297352543	8.92341	-55.6798104	3085.3
-0.05	-0.4	-0.488578445	0.01672	-0.350847068	0.00242	-0.722165803	0.20197	-0.349087918	0.00259	-0.852331709	0.27	-0.348230149	0.00268
-0.025	-0.4	-0.418126228	0.00074	-0.352001294	0.0023	-0.652506183	0.1068	-0.35028507	0.00247	-0.858852692	0.22116	-0.350029255	0.0025
0	-0.4	-0.534214056	0.0201	-0.35379939	0.00213	-0.594126218	0.04485	-0.350801733	0.00242	-0.750497318	0.15288	-0.352496773	0.00226
0.025	-0.4	-0.403800953	1.44E-05	-0.453222104	0.00283	-1.456809045	1.77995	-3.895485908	15.5166	-1.392655203	2.82702	-5.408043408	31.1053
0.05	-0.4	-2.627670158	4.96251	-72.63265084	5217.56	-2.988393793	9.27955	-78.87878808	6164.29	-8.478286505	-281.66	-0.05942798	0
-0.05	-0.3	-0.318492049	0.00034	-0.269548151	0.00093	-0.619212462	0.14035	-0.27021482	0.00089	-0.724824892	0.25902	-0.268348556	0.001
-0.025	-0.3	-0.318096947	0.00033	-0.238163526	0.00382	-0.601228582	0.13005	-0.268903687	0.00097	-0.669440744	0.17694	-0.269101016	0.00096
0	-0.3	-0.482227929	0.05304	-0.273249073	0.00073	-0.530849929	0.06556	-0.269943125	0.0009	-0.663261131	0.1607	-0.268876438	0.00097
0.025	-0.3	-0.49326592	0.03735	-1.613540256	1.72539	-0.560717715	0.07445	-2.070350235	4.60969	-7.568568818	-646.05	-2.618133989	-392.822
0.05	-0.3	NA	NA	NA	NA	-2.048872199	3.55704	-44.16070439	1923.93	-15.82061612	-2782.9	0	0.09
-0.05	-0.2	-0.255677446	0.0031	-0.186483862	0.00018	-0.477466266	0.1074	-0.185540577	0.00021	-0.550501732	0.19284	-0.184895723	0.00023
-0.025	-0.2	-0.22897118	0.00084	-0.18632158	0.00019	-0.438867934	0.09278	-0.186122241	0.00019	-0.713536	0.33955	-0.185981573	0.0002
0	-0.2	-0.315832815	0.02199	-0.186925045	0.00017	-0.478403103	0.08323	-0.18638619	0.00019	-4.377669033	-242.13	-0.185943297	0.00122
0.025	-0.2	-0.361629157	0.02873	-0.186829064	0.00017	-5.444286093	-415.52	-0.192316826	0.0015	-6.18972513	-513.62	-0.198201168	0.00355
0.05	-0.2	-2.137854001	3.75528	-0.185399368	0.00021	-2.047270789	4.03034	-0.440469101	0.21727	-6.962226768	-513.19	-0.397243218	0.50808
-0.05	-0.1	-0.230492155	0.01703	-0.095758738	1.80E-05	-0.206791186	0.05203	-0.095914719	1.67E-05	-0.895809524	0.87858	-0.095441525	2.08E-05
-0.025	-0.1	-0.145746446	0.00209	-0.096342493	1.34E-05	-0.568115785	0.23192	-0.096202974	1.45E-05	-0.926331077	0.81616	-0.096447109	1.29E-05
0	-0.1	-0.25285078	0.02425	-0.096680592	1.10E-05	-0.628839606	0.29838	-0.096276225	1.39E-05	-0.555835468	0.32854	-0.097011201	1.06E-05
0.025	-0.1	-0.326825167	0.0521	-0.119200155	0.00126	-0.529192564	0.18605	-0.58452544	0.361	-4.350322056	-256.45	-0.400935286	4.76644
0.05	-0.1	-0.972888899	0.77963	-0.92410646	0.69275	-4.81041703	-402.6	-1.8602238	433.871	-15.30080204	-2012.8	-5.180290476	-107.577

Table 3. A table showing the median and MSE for eta for both estimation methods for all of the 271 converging conditions. Trend was not a significant factor in estimating eta, so it was averaged over. Cells marked with "NA's" denote conditions for which there were not enough converging iterations to perform analysis.

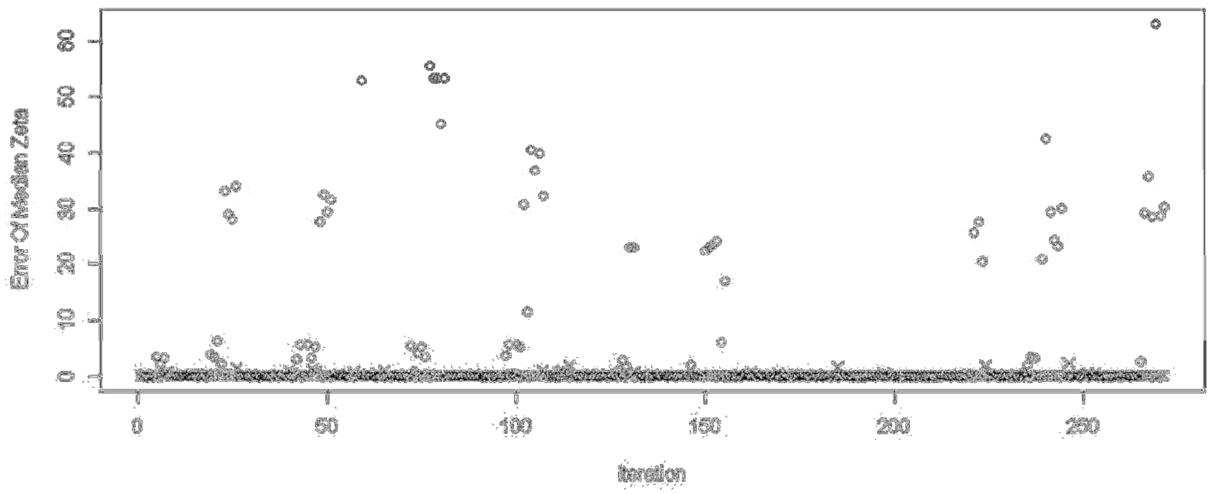

Figure 10. Plot depicting the error of the estimated median zetas for both estimation methods. The "X's" represent the higher-order derivative method, and the "O's" represent the LDE method. Each converging iteration is shown across the x-axis.

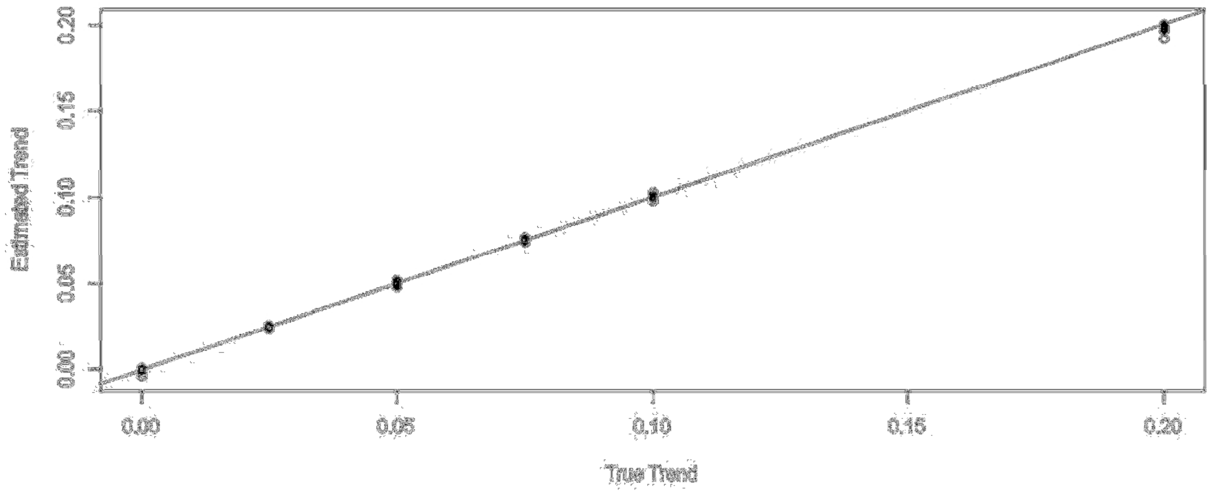

Figure 11. A plot of the true trend versus the estimated trend for all of the converging simulation conditions for the higher-order derivative method.